

Meeting title	CCP4 Working Group 2 meeting (chaired by Arnaud Basle, University of Newcastle)		
Date	Wednesday 11th of September 2024	Time	10.00 – 12.00
Location	Virtual only	Zoom	yes
Circulation	ccp4wg2@stfc.ac.uk		
Attending online	Jon Agirre, Arnaud Basle, Elke de Zitter, Deborah Harrus, Karen McIntyre, Clemens Vonnrhein, Airlie McCoy, Filipe Menezes, Petr Kolenko, Dave Briggs, Ivo Tews, Julian Wills, Keitaro Yamashita, Luiso Fuentes Montero, Martin Maly, Melanie Vollmar, Robbie Joosten, Marcin Wojdyr, Ville Uski, Charles Ballard, Andrey Lebedev, Hannah Kwon, Briony Yorke, Stuart McNicholas, Victoria Burge, Paul Bond, Ronan Keegan, Ralf Flaig, Eleanor Dodson, Mark Roe, Keith Wilson, Dorothee Liebschner, Paul Rowland.		
Apologies from			

10.00 Welcome

10.05 Chair's update

Last meeting's minutes: these were circulated and amended shortly after the last meeting. We hear no complaints, so the minutes are accepted 

10.15 Northern meeting

Meeting happening at the Frederick Douglass Centre in Newcastle. Nice big venue. Organised by Arnaud and Vic Burge, with Briony Yorke and Jon Agirre overseeing the process. Working on a website.

Airlie has a comment on the Southern Summer School in Norwich:

Airlie McCoy to Everyone 10:06



FYI, We have just finished the southern school in Norwich. The 24 students were mostly international and excellent.

Airlie McCoy to Everyone 10:07



Thanks to Dave Lawson for organising, it worked very well at the JIC - first time there in person.




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10.35 CCP4 Study Weekend 2024 (Clemens Vonnrhein)

Clemens gives an overview of papers in process and accepted. Two from Global Phasing are well advanced. Clemens has seen another one to publication, another one from Garib is

nearly there, two other people said they were going to submit but haven't reacted to reminders,

There's a discussion around collecting papers as a virtual issue rather than printed. Melanie says that that is currently happening in IUCr Journals. Ivo suggests that related past papers could be collected into a virtual issue.

 **Airlie McCoy to Everyone** 10:11
This is continuing the pattern of it getting harder and later to get papers out of people. Do we need to rethink the idea of the proceedings. It is starting to get ridiculous

 **Airlie McCoy to Everyone** 10:15
How does 'credit to the meeting' work with past publications?

CHECK THE CHAT!!!

 **Melanie Vollmar to Everyone** 10:16
I guess this is more if it happens that a paper was in the works and going through peer-review (how ever long that takes) and then the topic is included in the SW then that could be linked rather than write a new one

 **Paul Bond to Everyone** 10:17
There was a previous decision made that publishing after the Study Weekend was optional, and you could say to the organisers that you were happy to present but didn't have an intent to publish. That sounds like that has now been reversed?

  ...

 **Airlie McCoy to Everyone** 10:18
Yes, I think the option was sort of approved. It was for the first speakers in the session who were presenting teaching talks

10.55 **CCP4 Study Weekend 2025 (Deborrah Harrus, Elke de Zitter, Dorothee Liebschner)**

“Using software, AI and other methods to advance crystallographic models.”

Here is a capture from Elke's slides outlining the meeting.

Using software, AI and other methods to advance crystallographic models

- Keynote lecture
 - Duration altered as compared to last year: 45 minutes
- Panel discussion
 - Duration: 45 minutes
- Sessions
 - 5 sessions with 3 speakers and total of 90 minutes
 - 1 session with 4 speakers and total of 100 minutes

The panel discussion will cover the topic "Are we training structural biologists for jobs that won't exist?". Some people say it's depressing, some people say it's thought provoking, so it seems like the ideal topic for an engaging discussion.

 **Airlie McCoy** to Everyone 10:22
How do we train SB for jobs of the future

I would suggest that a speaker that will appear in person is preferable

Elke proceeds to discuss the possible names attached to the sessions.

Names are **omitted** from the minutes as the speakers are **not yet confirmed**.

A point is raised on the appearance of multiple overseas speakers on the programme:

 **Airlie McCoy** to Everyone 10:34
There used to be a limit of 2 from the USA

Is the budget increased?

 **Melanie Vollmar** to Everyone 10:34
Yes. Budget?

 **Karen McIntyre - STFC UKRI** to Everyone 10:35
I took over booking the flights which meant we could keep an eye on the cost

There is just one speaker who needs to do a remote talk.

Ivo suggests having a session on AI assisted structure design. A person named on the programme works on something related, Elke suggests asking that person to cover protein design. Ivo mentions that it would be interesting to see how this comes full circle, with people using AI to design proteins and then testing them experimentally.

MM Martin Maly iPhone to Everyone 10:45

We may consider to include a 30 minute talk - introduction to crystallography - for students who are not familiar with standard methods. There are many of them usually.

[Collapse all](#) ^

ED Elke De Zitter 10:47

We specifically asked the speakers to introduce their topic well so that also new crystallographers can follow. We haven't included a "introduction to crystallography" talk.

To finish, some key facts on the meeting:

Key facts

Dates: 7-9 January 2025

Venue: EMCC, Nottingham, UK & Hybrid

Assuming 250 in person delegates

Key dates:

Registration opens: ? September 2024 – aim for 13th

Travel bursary applications close: 31 October 2024

EB registration closes: 11 November 2024

Registration for in-person event closes: 6 December 2024 (or earlier if places sell out)

Registration for virtual event closes: 9 January 2025



Minutes



12.55 Any other business

Ivo has something to add on the progress of the CoSec.

There is a proposal that Ivo is preparing. Looking at new ways to implement code (e.g. GPU accelerated MR). Involving CCP-EM, CCP-Biosim and CCP-N. Community building activities (e.g. meetings) can access a large pot.

 **Keith Wilson** to **Everyone** 10:46
Can you give us the title of the other work packages?

The next meeting will be in person, and we'll discuss a number of software developments. Tentative agenda and Doodle poll to follow – stay tuned and see you soon!